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Global calibration of ecological models for planktic foraminifera from coretop carbonate oxygen-18

Gavin A. Schmidt

NASA Goddard Institute for Space Studies and Center for Climate Systems Research,
Columbia University, New York

Stefan Mulitza

Department of Geosciences, University of Bremen, Bremen, Germany

Abstract

A global dataset of coretop planktic foraminiferal $\delta^{18}\text{O}_c$ is combined with a global database of seawater $\delta^{18}\text{O}_w$ observations and ocean climatologies to determine robust optimum parameters for an ecological model for six commonly measured species and varieties. These parameters consist of the temperature ranges, optimum temperatures, depth habitat, and the amount of secondary calcification for *G. ruber* (white), *G. ruber* (pink), *N. pachyderma* (l), *N. pachyderma* (r), *G. sacculifer*, and *G. bulloides*. This approach produces ecological models and temperature ranges consistent with previous work, and manages to reproduce the coretop oxygen-18 carbonate values remarkably well. The standard error of modelled values of coretop calcite globally and for all species is 0.53‰, compared to an error of 1.2‰ when assuming annual average mixed layer equilibrium calcite.

KEYWORDS: planktic foraminifera, seawater $\delta^{18}\text{O}$, carbonate $\delta^{18}\text{O}$, marine sediments

1. Introduction

The measurement of oxygen isotope ratios¹ in foraminiferal carbonate found in marine sediments remains one of the most quantitative and widespread records of past climatic changes. However, the signals that are recorded are integrated measures of a multiplicity of factors (the local temperature, the global ice volume, water mass changes, behavioural or ecological variation of the foraminifera and selective dissolution and bioturbation in the sediments themselves). Determining the relative importance of these factors is essential to improving our interpretation of any particular temporal or spatial pattern.

This paper attempts, for the first time, to use global databases of coretop $\delta^{18}\text{O}_c$ measurements and seawater $\delta^{18}\text{O}_w$ measurements to calibrate the ecological parameters governing the net isotopic signal of four commonly measured species and two varieties. While this approach has been used on individual locations [e.g. *Fairbanks et al.*, 1982] no previous attempt has been made to quantify the isotopic behaviour of foraminifera at the global scale. There are many more locations with coretop data and $\delta^{18}\text{O}_w$ profiles than there have been specific observations of the ecology of these species. By combining the two abovementioned new databases, we hope to be able to significantly increase the geographical range over which these parameters can be tested.

These data could be used in one of two ways. Firstly we could assume a particular depth habitat for each species (i.e. the mixed layer), and then use the data to calibrate a temperature dependent fractionation curve for the coretop isotopic values. However, we know that species have temperature-related preferences, that they can accrete carbonate at multiple depths, and are subject to dissolution effects in the sediment. Hence any resulting calibration is unlikely to be valid over a wide range of climatic, geographic or temporal variation. Alternatively, and this is the approach adopted here, we assume that we know how calcite fractionates, and we use the data to discriminate between plausible ecological models that include

many of the factors that are known to play a role. This has the advantage of allowing us to input the maximum amount of prior information, and increases our confidence that the resulting models will be of more general use. Thus we hope to optimise a set of ecological parameters for each species that gives us the widest possible predictive capacity.

Observations of these species in situ using sediment traps and full depth profiling [e.g. *Deuser*, 1987; *Deuser and Ross*, 1989; *Sautter and Thunell*, 1989, 1991] have guided all of the choices made here. Thus this work should be seen as trying to extend the observational data to encompass the entire core-top repository. The results may differ in various details, but that is due to trying to produce the most generally applicable parameters.

The utility of these ecological models is for the 'forward modelling' of carbonate data i.e. estimating the species-specific isotopic signature in the sediment as a function of the oceanographic/climatic conditions. Changes in those conditions could be drawn from a complex numerical simulation of any particular climate event or time-slice, or simply from hypothesised variations in the hydrographic profiles. Hopefully this may subsequently prove useful for the interpretation of down-core variability. However, we stress that an inversion of these models to get a surface temperature and/or $\delta^{18}\text{O}_w$ given a number of measurements of $\delta^{18}\text{O}_c$ from co-existent species is an under-determined problem. That is to say, there may be more than one solution consistent with the sediment isotope values.

One complication that arises is that the correct temperature dependence of fractionation is poorly understood. Hence the numerical experiments described here were all performed with a range of equations derived from different methodologies. Details are given in the ecological model description while the difference this makes is described for each species in the results section.

2. Summary of coretop database

The data used here is a subset of a global compilation of coretop data for the most commonly used species of planktic foraminifera (*Globigerinoides ruber*, *Globigerinoides sacculifer*, *Globigerinoides bulloides*, and *Neoglobobulimina pachyderma*) and their common varieties [Mulitza, 2001]. This compilation comprises more than 2500 measurements from published and unpublished sources. The shell sizes range from 150 to 600 μm . However, most of the mea-

¹Isotope values are given using the standard " δ permil" notation defined as

$$\delta^{18}\text{O} = \left(\frac{R_{\text{sample}}}{R_{\text{standard}}} - 1 \right) \times 1000$$

where $R = \text{H}_2^{18}\text{O}/\text{H}_2^{16}\text{O}$. Vienna standard mean ocean water (VSMOW) is used as the standard for seawater $\delta^{18}\text{O}_w$, Pee Dee Belemnite (PDB) is used as the standard for carbonates $\delta^{18}\text{O}_c$.

measurements are in the range often used for down-core studies (250–400 μm). The published part of the data set is partly based on previous compilations. Because some of the compilations used the same sources, we carefully checked the data set and eliminated double values. About 50% of the measurements were performed in the labs of the University of Bremen and the Alfred-Wegener-Institute for Polar and Marine Research in Bremerhaven. Both labs are closely intercalibrated and use the same preparation technique for stable isotope analyses of carbonates [e.g. *Mulitza et al.*, 1998]. These measurements were exclusively performed on foraminifera from sediment surfaces recovered with box- and multicorer devices. The entire data set including the references is available from the Pangaea data base (<http://www.pangaea.de/home/smulitza/>).

From the point locations of the coretop data, a $4^\circ \times 5^\circ$ gridded version of the data set was produced for each species. For each gridpoint, all coretop locations within a radius of 5 degrees are averaged using a weighting that gives most weight to the points nearest the gridpoint centre. This produces a sparse field (gridpoints further than 5 degrees away from nearest coretop are not set) that contains most of the structure, without over-interpreting the data.

Possible problems in the data exist because of cross-calibration issues between different laboratories, and possible confusion of present-day and Last Glacial Maximum (LGM) shells in areas with low sedimentation rates (which would tend to give higher $\delta^{18}\text{O}_c$ values). Additionally, any sediment focusing from areas with significantly different temperature structures will give a misleading average value. Partial dissolution of calcite, particular in the Pacific may also complicate the issue. While these possible errors are not corrected for, the large number of coretops used should serve to minimise their influence on the results.

3. Summary of $\delta^{18}\text{O}_w$ data

The global oxygen-18 database [*Schmidt et al.*, 1999; *Schmidt*, 1999b; *Bigg and Rohling*, 2000] is a database of about 15,000 observations of seawater oxygen-18 from all over the globe and from all types of marine environment. Much of this data comes from different laboratories, with different standards and techniques, and so the cross-calibration of the data is a necessary task. This is done using the GEOSECS measurements [*Östlund et al.*, 1987], which covered all three ocean basins and most types of open ocean

environment, as a benchmark or 'gold standard' to which all other measurements can be compared. If a known deep water mass (that we assume to be stable over the last few decades) has an isotopic value significantly different from the GEOSECS value for the equivalent water mass, a constant offset was applied to that source of data in order to bring it into line. This results in significant offsets to a number of data sets, but can only be applied to data that included deep water measurements. Data sets that only included measurements for the upper ocean were simply screened for any obvious inconsistency with any neighbouring data.

A vertical profile is used if there are at least 2 points in the vertical, with the first point above 50m and the last point below 100m. Clearly these profiles vary widely in quality, however, 60% of the over 600 profiles have 10 or more points in the vertical. The profile is then linearly interpolated onto the upper 13 levels (0, 10, 20, 30, 50, 75, 100, 125, 150, 200, 250, 300, and 400 meters) used in the temperature and salinity climatologies [*Levitus et al.*, 1994]. In the region of the thermocline, this can cause some significant errors. However in the absence of better data, this is unavoidable. Subsequently, a similar procedure to that used for the coretops is used to create a horizontal $4^\circ \times 5^\circ$ gridded data set of $\delta^{18}\text{O}_w$. Since the gridded data is sparse, the gridpoints with $\delta^{18}\text{O}_w$ information will not in general match the gridpoints with coretop data. However, some areas that have been well-sampled both for $\delta^{18}\text{O}_w$ and $\delta^{18}\text{O}_c$, in particular, the higher latitudes (the Arctic Ocean/N. Atlantic, the Southern Atlantic) and the Indian Ocean. For lack of any significant seasonal data, we assume that this dataset represents an 'annual' average.

We have made a conscious decision not to estimate $\delta^{18}\text{O}_w$ values on the basis of salinity/ $\delta^{18}\text{O}_w$ relationships because they vary significantly with region, and it is unclear whether these relationships are even stable over the seasonal cycle (since that has rarely been measured) [*Schmidt*, 1999a].

4. Ecological model parameters

The ecological models that we are trying to derive are relatively simple, and should be seen as a primitive attempt to quantify the temporal and vertical weighting of the carbonate that forms in the sediment. This weighting is essentially the percentage of carbonate found in the sediment that was calcified at a particular depth, at a particular month. Fortunately, the

absolute amount of carbonate does not affect the isotopic signal (other than the obvious, where there is zero abundance, there is no isotopic signal to match). Hence, much of the complication of nutrient and carbonate cycles can be neglected.

This approach has been introduced in a previous study [Schmidt, 1999b], but the extent of coretop data against which it was tested was limited. With the added information included here, more statistically valid measures can be used to discriminate between possibilities.

For each gridpoint, equilibrium calcite values are calculated for each vertical level, and for each month. For the base experiments, the equation used to estimate the equilibrium calcite value is derived from inorganic calcite experiments [Kim and O’Neil, 1997, hereafter KO97]. However, we have also examined the results using different equations based on cultures [Erez and Luz, 1983, hereafter EL83] and in situ calibrations [Mulitza *et al.*, 2002, hereafter M02] (Table 1). At warm temperatures, EL83 and KO97 are similar, while M02 is about 0.5‰ more depleted (and in fact similar at high temperatures to more recent culture experiments with *G. bulloides* [Bemis *et al.*, 1998, Equation 4]). At lower temperatures M02, KO97 and EL83 are more similar. These variations in the calcite value for the same temperature can make a significant difference. For example, an equation that produces a more depleted calcite value will generally give rise to an ecological model parameters that imply a preference for cooler/deeper water masses. Some of the main differences are pointed out in the text.

One possible factor in this confusion may be due to the carbonate concentration effect estimated (experimentally and theoretically) to be about -0.002‰ kg/ μ mol [Spero *et al.*, 1997; Bemis *et al.*, 1998; Zeebe, 1999]. Since surface carbonate ion concentrations are quite well correlated with temperature in the global ocean [CO_3^{2-}] = 104. + 6.4*T* (standard error, = 29 μ mol/kg, r^2 = 0.79) [Östlund *et al.*, 1987], field calibrations will implicitly include this effect, while culture or inorganic calibrations will not.

Initially, this effect was neglected (i.e. we assume constant values globally). However, in an attempt to partially correct for this factor, we also performed some experiments using KO97 including a correction factor of $-0.002(104. + 6.4T - C_0)$ ‰, where C_0 is an estimate of the carbonate concentration used in the KO97 experiments. This was not reported in that study, but we estimate that it must have been close to

the saturation value between 50 and 70 μ mol/kg. We take $C_0 = 60 \mu\text{mol/kg}$ as a rough estimate. Using this correction gives about -0.44‰ at 28°C, which almost exactly matches the offset between M02 and KO97 at this temperature. The error in this estimate is about ± 0.05 ‰ and is a function of the accuracy of the regression, our estimate of C_0 and the accuracy of the carbonate ion effect. However, since this new equation closely matches that of M02, the results obtained are rather similar, and thus are not described further. There may of course be other reasons why the inorganic calcite laboratory results differ from both the culture experiments and in situ calibrations, and so this estimated correction should be seen merely as one possibility.

Another factor that affects the calcification for symbiotic species (such as *G. ruber* (white) and *G. sacculifer*) are light levels [Spero and DeNiro, 1987]. For instance, *Orbulina universa* and *G. sacculifer* have been shown to produce more depleted calcite under high light conditions [Spero and Lea, 1996; Bemis *et al.*, 1998]. This could lead to more enriched calcite at deeper levels (as light levels decrease). However, this effect is hard to calibrate for the vertical migrations of the species examined here, nor for the range of likely light levels in actual ocean situations and therefore is neglected for this preliminary study. Since light levels are correlated with depth, and thus temperature, neglect of this effect will tend to produce temperature preferences that are a little cool.

Whatever the calcite equation used, the ecological model must determine a weighting function in depth and time (over the year) for averaging these multiple values into a mass-weighted annually averaged value that could be expected to measured in the sediment.

The first constraint on the ecology is assumed to be temperature based. For each species, we assume that there exist a maximum (T_{max}) and minimum (T_{min}) local temperature beyond which the foraminifera will not survive/reproduce. These limits have been examined in previous work (based on culture experiments [Bijma *et al.*, 1990] or the global distribution of species [Vincent and Berger, 1981; Tolderlund and Bé, 1971]), but here will be determined by their effect these limits have on the $\delta^{18}\text{O}_c$. One minor validating test of this methodology will therefore be how closely our limits match those determined in other ways.

Secondly, within the range determined above, we assume that there is an optimal temperature (T_{opt}) at which the foraminifera is most abundant. This can be a very sharp peak, or rather broad, and hence we

introduce one other parameter, the standard deviation (assuming a normal distribution) of abundance with respect to temperature (σ_T) around the optimal peak (see Table 1 for details).

The next factor is the depth habitat of the species. Given the variation in mixed layer depth and thermohaline stratification in the oceans, any kind of constant depth assumption is clearly insufficient. Hence we define a number of derived values that characterise the stratification of the local water column (for instance, the mixed layer (ML) depth is defined as the depth above which the potential density is within 0.125 kg m^{-3} of that of the surface [Levitus *et al.*, 1994]). The pycnocline (PYC) depth is the point of maximum gradient in potential density and we define a deep chlorophyll maximum (DCM) as the minimum of the pycnocline depth and the maximum depth to which sufficient light for photosynthesis penetrates (assumed to be 80m globally). These depths will vary both temporally (over the seasons and inter-annually) and spatially. Combining the two temperature constraints with the depth habitat gives a relative abundance (which can be zero) of the calcite for each month.

Note that a number of species give higher (more enriched) isotopic values for specimens taken from the sediment compared to those taken from the surface ocean. These differences could be due to a number of factors: secondary calcification below the thermocline, growth rate or temperature related vital effects combined with selective dissolution [Duplessy *et al.*, 1981], or the effects of bioturbation bringing up glacial age specimens. For those species that have an observable amount of secondary calcite (such as *G. sacculifer*) and are possibly subjected to selective dissolution while in the sediment [Lohmann, 1995], the fraction of secondary calcite (F_{post}) is also a free parameter (we choose discrete values for this parameter 0, 10%, 20%, etc.). We assume that the secondary calcification occurs below the thermocline, with a maximum depth to be determined. Combining this with the primary calcite, then gives an average isotopic value in the sediment typical for an entire year.

Table 1 summarises the free parameters in the ecological model. Since this is a multi-parameter problem, with a model that is not easily amenable to partial differentiation, we have chosen to use a Monte-Carlo-like method to estimate the best fit. Hence, for each species, (and within a few loose a priori constraints based on previous work), a large number of sets of possible parameters are tested. For

each set of parameters, a separate numerical simulation is performed and the simulated coretop values compared with the observations. The parameter set that gives the minimum error over all the points where they match the coretop data is deemed to be the best. Specifically, the optimal set of parameters is defined as the one that give a maximum value of $\Gamma((N - M)/2, \chi^2/2)$ where N is the number of coretops, M is the number of free parameters in the ecological model, and $\chi^2 = \Sigma^N (y_i - y(x_i))^2 / \sigma^2$ is measure of the overall error. Since we can only have an estimate of σ (the measurement error (small) combined with sampling errors over time and space (unknown)), the Γ values do not provide an absolute measure of the goodness of fit (even between species), but merely provide a scale against which to test the models. Since different models match varying numbers of coretops, this measure is more robust than simply looking for the minimum χ^2 [Press *et al.*, 1990]. Technically, Γ gives the rough probability that our model could have produced the observed distribution (given the estimate of measurement errors). Due to the uncertainty in the measurement and sampling errors, and also to the non-linearities of the model parameters, it is not an absolute probability. A related quantity σ_E , the standard error of our model, is given by $\sigma_E^2 = \Sigma^N (y_i - y(x_i))^2 / (N - M)$.

As an example, fig. 1 shows the 'goodness of fit' for various sets of parameters for one particular species (*G. sacculifer*). For each set, each parameter is plotted against Γ (for graphing convenience, F_{post} has been plotted as $-F_{post}/10$). The 'best-guess' can be read off the graph as the points furthest to the right for each parameter.

This procedure does not necessarily guarantee sensible results. Where the matching coretops do not fully sample the range of habitats for a species, the minimization procedure can sometimes lock on to a set of parameters that simply minimises the error for a few exceptional points. Another feature of this procedure is that occasionally coretops at the edge of a particular species domain can be included or excluded in the match as a function of the minimum and maximum temperatures. If the excluded coretop is an outlier, the Γ for that set of parameters may be greater than if it were included. Consequently, we have tried to maximise the number of coretops included in the match, and so we have used maximum and minimum values of temperature accordingly, regardless of whether a slightly better correlation can be gained by dropping a couple of outliers.

Given the problems in the different data sets and the amount of vertical, and seasonal interpolation that is necessary, these optimised models are likely to be only roughly correct. That they seem to end up with similar temperature tolerances and species ranges that have been seen in the literature, gives us some confidence that the process is valid. Precise error bars on the parameters are however difficult to determine.

Some aspects of ecological behaviour are clearly not captured by this model. Ocean depth profiles that are more complicated than the mixed layer-thermocline-deep ocean picture implicitly used above (for instance, the areas of the Arctic where there is a cold halocline layer above warmer Atlantic water) could lead to different depth abundances for species that would not be well captured.

5. Results

For each species the optimal set of parameters to the coretop data are summarised in Table 2. Two panels are illustrated for each species (i.e. *G. ruber* (white) in fig. 2). The first shows the observed coretop values for the species and is sparse due both to limited sampling and the regional distribution of the species. For reference, the standard error for a generic model for the annual average surface equilibrium calcite using the observed surface $\delta^{18}\text{O}$ have also been calculated (σ_{seq}). In every instance, this is less good at explaining the coretop values than the optimal parameters.

The calculated coretop value for all the grid points where water profile observations exist is shown on the second panel. This is also sparse due to limited sampling, and also due to the temperature constraints in the ecological model (i.e. if the temperatures are outside the range for the depth habitat of a particular species, no calcite will be produced and no isotopic value is given). When comparing the panels, two factors should stand out - the match of the distribution, and the actual values of the coretops. While the latter factor has been tuned for (and is the basis of the method), the predicted distribution is only indirectly constrained and hence serves as an extra validation test. Note that the model cannot know that a particular species has a particular habitat in the Atlantic, but is completely absent in the Pacific (for instance, *G. ruber* (pink) or *G. ruber* (white)).

As can be seen from the figures, the number of coretops used in this procedure varies enormously from

over 300 for *N. pachyderma* (l), to barely 25 for *N. pachyderma* (r). Consequently the power of the optimised model will also vary. However, in order to test robustness of the procedure we also do separate minimisations on each geographically separated population (i.e. the Indian and Atlantic Ocean populations of *G. ruber* (white), or the Northern and Southern Hemisphere populations of *N. pachyderma* (l)). If the optimal parameters are essentially the same in each case, we can have increased confidence in the results.

5.1 *G. ruber* (white)

G. ruber (white) is known to be a tropical mixed layer species with a distribution mainly in the Atlantic and Indian oceans. Unfortunately, the tropics are particularly poorly sampled for $\delta^{18}\text{O}_w$. Hence the number of matches of coretops and isotopic profiles is small (65). Nevertheless, the match in fig. 2 is quite good. Previous work on its temperature tolerances in culture indicate a tolerance of $14^\circ - 32^\circ$ [Bijma *et al.*, 1990], which is almost exactly replicated in this analysis. Here we find that using the KO97 equation, the optimum tolerance is $13^\circ - 32^\circ$, and an optimum temperature of 32° with a standard deviation of 14° (i.e. there is higher abundance at higher temperatures, but the peak is very broad). The standard error for this set of parameters is about 0.44, which is lower than the $\sigma_{seq} = 0.52\text{‰}$ for annual average surface equilibrium calcite model.

If we use different equilibrium calcite equations (EL82, M02), the results do vary (for EL82, $T_{opt} = 31$, $\sigma_T = 7$ and for M02, $T_{opt} = 14$, $\sigma_T = 8$) but are not as significant ($\sigma_E = 0.49, 0.52$ respectively), indicating that KO97 is a more valid calculation, at least for this species. Looking only at the Atlantic coretops gives identical results for all the calcite equations.

There is some indication that *G. ruber* (white) specimens in sediment are more enriched in $\delta^{18}\text{O}_c$ than those in the surface waters [Duplessy *et al.*, 1981]. However, this species is not thought to accrete secondary calcite, and so this could be related to some kind of selective dissolution, or perhaps bioturbation of older sediments.

5.2 *G. ruber* (pink)

G. ruber (pink) is a related species to *G. ruber* (white) but has a markedly different ecological profile. In particular, there is strong evidence that *G. ruber* (pink) has a 'vital' effect that leads to the incorporation of light metabolic isotopes. Analyses of sediment

traps indicate that *G. ruber* (pink) isotope values can be significantly more depleted than equilibrium calcite at these locations [Williams *et al.*, 1981; Deuser and Ross, 1989].

For this procedure, there are not enough matching coretop data to provide robust results. Using KO97, the best parameter set has a range 16–31°, an optimum temperature of 30°, $\sigma_T=6^\circ$, giving $\sigma_E = 0.55$). Interestingly, using M02 (which predicts carbonate about 0.5‰ more depleted over this temperature range), the result is very different (range 17–31°, optimum 22°, $\sigma_T=4^\circ$, giving $\sigma_E = 0.42$). For reference, $\sigma_{seq} = 0.64$. Since the results with M02 are significantly better, we choose to illustrate those in fig. 3. However, since the implied distributions are so varied and significantly different from previous work [Bijma *et al.*, 1990; Tolderlund and Bé, 1971], further coretops (only 31 were matched here) and/or more tropical water profiles will be needed to resolve this issue.

5.3 *G. sacculifer*

G. sacculifer is another tropical mixed layer species which appears in all tropical oceans. As for *G. ruber* (white), the number of coretop-profile matches are limited (56), however this does appear to be sufficient to determine a reasonably robust result (fig. 4). All coretop observations are of the specimens without a final sac (i.e. *G. sacculifer trilobus*). This species accumulates a secondary layer of calcite during gametogenesis which has been estimated at about 20–30% by weight [Lohmann, 1995; Lea *et al.*, 2000]. The analysis here confirms that range, giving most likely estimates of 20% and 30%. However the difference in Γ between 20 and 30 per cent is very small and thus the procedure does not significantly distinguish the two cases ($\sigma_E = 0.44$ in both cases compared with $\sigma_{seq} = 0.61$). The optimum temperature of 21–23° and a $\sigma_T = 3$ –4 are consistent with previous results [Bijma *et al.*, 1990] but are possibly on the cool side.

With the EL83 equation, the results are identical, except that the percentage of secondary calcite is estimates to be only 10%. The errors are only slightly higher ($\sigma_E = 0.45$). Similarly to *G. ruber* (white), the use of the M02 equation leads to parameter sets that are significantly less accurate ($\sigma_E = 0.62$) and with a large negative mean offset of about -0.4‰.

Calcification for this species has been shown to be more depleted as light levels increase [Spero and Lea, 1993]. This implies that deeper (darker) calcite will be slightly more enriched than that formed at the surface. This will have the effect of increasing

the difference between surface and deep calcite in the same sense as for the carbonate effect mentioned previously. Including this effect would most likely lead to a warmer temperature preference and maybe a slight decrease in the percentage of secondary calcite predicted. However, the details of how to model this effect for real world situations (where depth and growth rate related factors would need to be calculated) have not yet been quantified.

5.4 *G. bulloides*

G. bulloides has a very wide distribution ranging from the high latitudes to the Arabian Sea. However, there is increasing appreciation that the morphologically similar specimens found in the sub-tropics and high latitudes are possibly not from the same species [Darling *et al.*, 2000]. For this reason we split the coretops into distinct regional groupings, the Southern Ocean (sub-Antarctic) population, the Northern Atlantic population (incl. the Mediterranean), and the Arabian Sea population. The few coretops from the N. Pacific can be added to the northern high latitude group, but better results are obtained if they are left out (i.e. they do not follow the same pattern as the more numerous N. Atlantic coretops). Unfortunately, the both the N. Pacific and the Arabian Sea coretops are too few in number to provide an independent estimation of their specific ecological parameters, and since they are considered to be upwelling indicators in these regions, they may be responding to hydrologic features smaller than are resolved in these data sets.

With these restrictions, it is possible to find distinct results for the two main sub-groups. In the North Atlantic, the parameters obtained indicate a relatively warm temperature range (3–19°C), an optimum at about 10–12°C and with $\sigma_T=4$ –5. The standard error for this region is a very low 0.33‰, using 80 coretops (compare this to 0.82 for σ_{seq}). For the southern ocean population, the picture is significantly different. There (60 cores), the ecological preference is towards cooler water masses (range 1–17°C, optimum at 1°C, with $\sigma_T=7$). However, the error on these estimates is larger (0.79 ‰) and there is a rather large mean offset (the modelled values are about 0.46‰ systematically too low). Clearly, with these temperature ranges, no carbonate value is predicted in the Arabian Sea region with either set of results. In order, to illustrate these alternate results, the modelled carbonate shown in fig. 5 is taken from both sets, the N. Atl. parameters used for the N. Hemisphere results, and

the Southern Ocean values used in the S. Hemisphere. The N. Pacific values do not fit well with either set, but are not sufficient on their own to define another discrete set.

The differences between the parameter sets and sub-groups could be related to variations in species type, or to differences in environmental factors. Looking at the GEOSECS data, southern ocean carbonate concentration could conceivably be about $50 \mu\text{mol/kg}$ lower than the North Atlantic at a similar temperature (the sparsity of data makes it difficult to be conclusive). This would translate into about a 0.1‰ increase for southern ocean calcite compared with the North Atlantic. Hence the ecological models for the southern ocean population would tend to chose a cooler preference to compensate (as observed). However, the fact that the temperature range (as opposed to the optimum) also seems cooler, possibly points to an actual ecological difference in addition to a carbonate related shift. Further work with more detailed estimates of the carbonate concentration is necessary to resolve this issue. Alternatively this species could calcify in a species dependent way, and require a different equilibrium calcite equation. However, none of the relevant equations from *Bemis et al.* [1998] lead to an improved fit. Size related features and possible vertical migration of this species as it matures could also play a role in explaining these discrepancies [*Spero and Lea*, 1996].

5.5 *N. pachyderma* (l)

N. pachyderma (l) is a high latitude species that is found at both poles, and appears to have a relatively homogeneous genotype between the isolated populations [*Darling et al.*, 2000]. Fortunately, the coverage of coretops in the high northern latitudes and the distribution of isotopic seawater profiles match to a very large extent. Hence, the number of coretops available for this analysis are very significant (313). We analysed the coretops globally, and also by taking each hemisphere separately.

A number of features stand out in the analysis. Firstly, note that the best results for *N. pachyderma* (l) occur when it is assumed to be a mixed layer species that has a significant amount of secondary calcite (which has been observed to be up to 75% in some locations [*Kohfeld et al.*, 1996]). This is in seeming contradiction to numerous studies that indicate that *N. pachyderma* (l) is slightly deeper dwelling (ie. in the deep chlorophyll maximum (DCM)). Possibly, our definition of the DCM or the vertical res-

olution of the isotopic profiles are not sufficient to differentiate between these cases. This is clearly an avenue deserving of further study. Nevertheless, the predicted isotopic values, and distribution in fig. 6 seem remarkably good. In particular, the distribution in the Arctic is clearly captured. The decrease in isotopic values in the Canadian Basin has been the subject of some speculation, but in this analysis, it is due mainly to the amount of depleted river runoff in the surface layers of the Arctic.

The standard error is about 0.5‰ globally for the optimal parameters ($-2-9$, $T_{opt} = 3$, $\sigma = 3$), but small differences from this do not increase the error appreciably. For reference, $\sigma_{seq} = 1.65$.

Difference between analyses on each polar population do not reveal any large inconsistencies, although there is a small tendency towards deeper dwelling in the southern ocean. For the other equations, EL83 produces very similar results, while M02 does significantly worse.

5.6 *N. pachyderma* (r)

N. pachyderma (r) has a much more restricted distribution than *N. pachyderma* (l), and generally appears equatorward of *N. pachyderma* (l) populations (fig. 7). However, the number of coretops with isotopic analyses of *N. pachyderma* (r) that match the seawater isotope profiles are very limited (25). Hence of all the species considered here, *N. pachyderma* (r) is the most poorly defined.

The best results come from a mixed-layer habitat with a temperature range of $1-13^\circ\text{C}$, an optimum of 10° and $\sigma_T = 3-4$. The standard error for these parameters is 0.64 (compared to $\sigma_{seq} = 0.97$). Additional secondary calcite, changes in the depth habitat (ML to DCM), and different calcite equations do not improve the fit. However, as with *G. ruber* (pink), the number of coretop matches are too limited for a robust appraisal of the ecology of this species.

6. Discussion

Understanding the ecological effects on the sedimentary isotopic record is a necessity if downcore variations are to be correctly interpreted. This study is the first attempt at creating globally calibrated ecological models for 6 separate species and varieties, with the aim of providing a forward model that takes any particular temperature, salinity and water isotope profile and predicts the species-specific coretop isotopic value. Since the resulting coretop value is

not unique, the inverse problem (i.e. what were the vertical hydrological profiles given a particular isotopic value) is highly under-determined. Possibly with more species that live further down in the water column (such as *G. truncatulinoides*), a combination of species may provide enough independent information to estimate some kind of stratification. However, the most effective use of these ecological models is probably in combination with ocean and coupled isotope general circulation models in order to estimate the sedimentary carbonate isotope response to various climate forcings (such a large meltwater event, or to conditions typical of the LGM).

We found that overall, the most accurate results were found when we used the KO97 calcite equation (with the exception of *G. ruber* (pink)). This is peculiar since it might be expected that a field calibration of surface dwelling specimens (such as M02) would be more accurate (since it takes into account any possible carbonate ion effect to the extent that this correlates with the temperature). This either points to a missing feature (or features) in our model (possibly some kind of selective dissolution or light level effect), or possibly a systematic bias in the conditions under which recent samples calcified compared to those in the coretops (i.e. due to recent (last few hundred years) temperature or carbon dioxide related effects).

In conclusion, using the optimal model for each of the species, the quality can be seen in fig. 8. The standard deviation over all species and for the whole range of carbonate values is 0.53‰ over 613 matching points. If we compare this to the 'null hypothesis' and simply use the surface equilibrium calcite value (derived from surface observations of $\delta^{18}\text{O}_w$ Levitus mean annual temperature and the KO97 temperature equation), then the correlation is much poorer with a standard error of about 1.2‰ (over 970 matching points).

A number of features of this procedure still need to be improved. In particular the interaction of the isotopic signal and the carbonate environment (i.e possibly relating the percentage of secondary calcification and dissolution to local hydrological conditions, such as the depth of the lysocline) and the effect of carbonate on the equilibrium fractionation needs to be better accounted for. Since carbonate concentrations have been infrequently controlled for, this factor is possibly also implicated in the differences seen between the various equilibrium calcite equations.

Also, the seasonality of the seawater isotopic values has not been included for lack of appropriate

data over most of the oceans. Some attempt to estimate these effects may improve the model. In addition, isotopic data from sediment traps and other foraminiferal proxies such as Mg/Ca ratios [Lea *et al.*, 2000] should be incorporated to give better constraints on the amount of secondary calcification and dissolution that occurs. A better classification of water density structure as a function of water mass [Fairbanks and Wiebe, 1980] could also be an advantage.

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- S. Mulitza, Department of Geosciences, University of Bremen, Bremen, Germany (smulitza@uni-bremen.de)
- G. A. Schmidt, NASA Goddard Institute for Space Studies and Center for Climate Systems Research, Columbia University, 2880 Broadway, New York, NY 10025 (gschmidt@giss.nasa.gov)

Table 1. Ecological model parameters and abbreviations

Parameter	Description
T_{max}	Maximum temperature tolerated ($^{\circ}\text{C}$)
T_{min}	Minimum temperature tolerated ($^{\circ}\text{C}$)
T_{opt}	Optimum temperature (greatest abundance) ($^{\circ}\text{C}$)
σ_T	Standard deviation of abundance ($^{\circ}\text{C}$) ^a
F_{post}	Percentage of secondary (sub-thermocline) calcite (%)
ML	Mixed layer depth (m)
PYC	Pycnocline depth (m)
DCM	Deep chlorophyll maximum depth ($=\min(\text{PYC}, 80)$) (m)
KO97	Equilibrium calcite using the <i>Kim and O'Neil</i> [1997] inorganic calcite equation ^b $T = 16.1 - 4.64(\delta^{18}\text{O}_c - \delta^{18}\text{O}_w) + 0.09(\delta^{18}\text{O}_c - \delta^{18}\text{O}_w)^2$
EL83	Equilibrium calcite using the <i>Erez and Luz</i> [1983] cultured foraminifera equation ^c $T = 17.0 - 4.52(\delta^{18}\text{O}_c - \delta^{18}\text{O}_w) + 0.03(\delta^{18}\text{O}_c - \delta^{18}\text{O}_w)^2$
M02	Equilibrium calcite using the <i>Mulitza et al.</i> [2002] field calibration from plankton tows and water samples at 3.5m depth ^b $T = 14.3 - 4.34(\delta^{18}\text{O}_c - \delta^{18}\text{O}_w) + 0.05(\delta^{18}\text{O}_c - \delta^{18}\text{O}_w)^2$

^aThe abundance within the range T_{min}, T_{max} is set to $\exp(-(T - T_{opt})^2 / 2\sigma_T^2)$, scaled so that the integral over the range is unity. σ_T is constrained so that the difference in weighting over the temperature range does not vary by more than a factor of ten.

^bThe appropriate conversion from VSMOW to PDB is $\delta_{PDB} = \delta_{VSMOW} + 0.27$

^cThe appropriate conversion from VSMOW to PDB is $\delta_{PDB} = \delta_{VSMOW} + 0.22$

Table 2. Optimal ecological model parameters

Species	Depth Habitat	T_{min} $^{\circ}\text{C}$	T_{max} $^{\circ}\text{C}$	T_{opt} $^{\circ}\text{C}$	σ_T $^{\circ}\text{C}$	Secondary Calcification		No. of matching coretops
						F_{post} %	Depth Range (m)	
<i>G. ruber</i> (white)	ML	13	32	32	14	-	-	65
<i>G. ruber</i> (pink)(KO)	ML	16	31	27	6	-	-	31
<i>G. ruber</i> (pink)(SM)	ML	17	31	22	4	-	-	31
<i>G. sacculifer</i>	ML	18	30–31	21–23	3–4	20–30	PYC	56
<i>N. pachyderma</i> (l)	ML	-2	8–9	3	2–3	50	PYC-400	313
<i>N. pachyderma</i> (r)	ML	1	13	10	3–4	-	-	25
<i>G. bulloides</i> (N. Atl.)	ML	3	19	11	4	-	-	80
<i>G. bulloides</i> (S. Hemi.)	ML	1	17	1	7	-	-	60

*Where we do not consider the results to be statistically different, a range is indicated

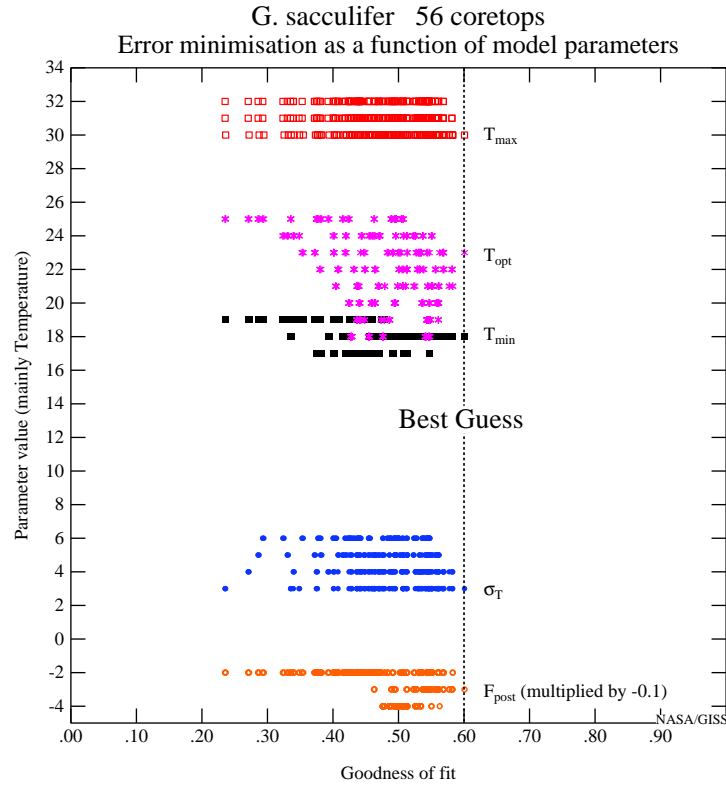


Figure 1. The variation of the goodness of fit as a function of model parameters for *G. sacculifer*. This is an example of the Monte Carlo technique that is applied for each species. The larger the goodness of fit, the more accurate the estimated coretop values. The 'best guess' values are those that are associated with maximum value (the points at the furthest right).

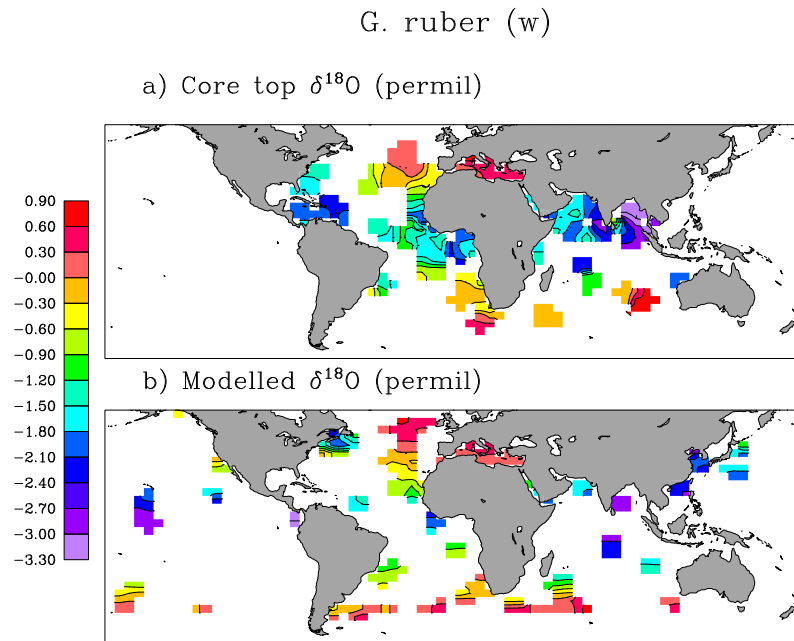


Figure 2. *G. ruber* (white). The distribution and isotopic value of (a) the observations of coretop carbonate, and (b) the predicted coretop carbonate based on the optimal ecological model for those points where hydrographic profiles exist.

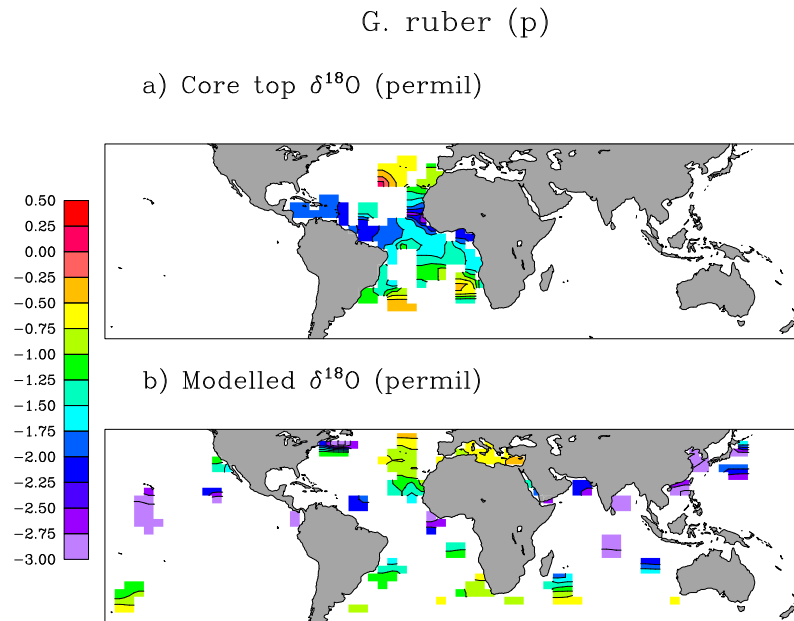


Figure 3. *G. ruber* (pink). Description as for figure 2.

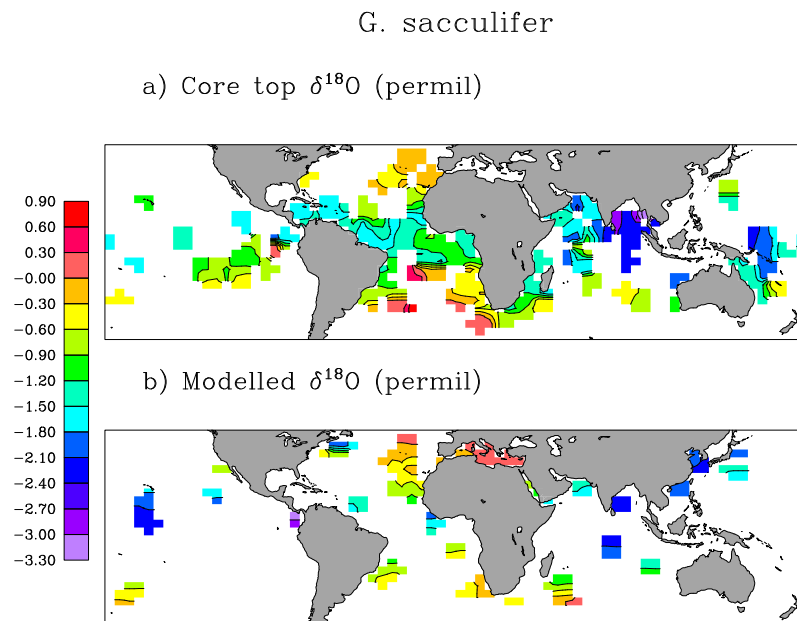


Figure 4. *G. sacculifer*. Description as for figure 2.

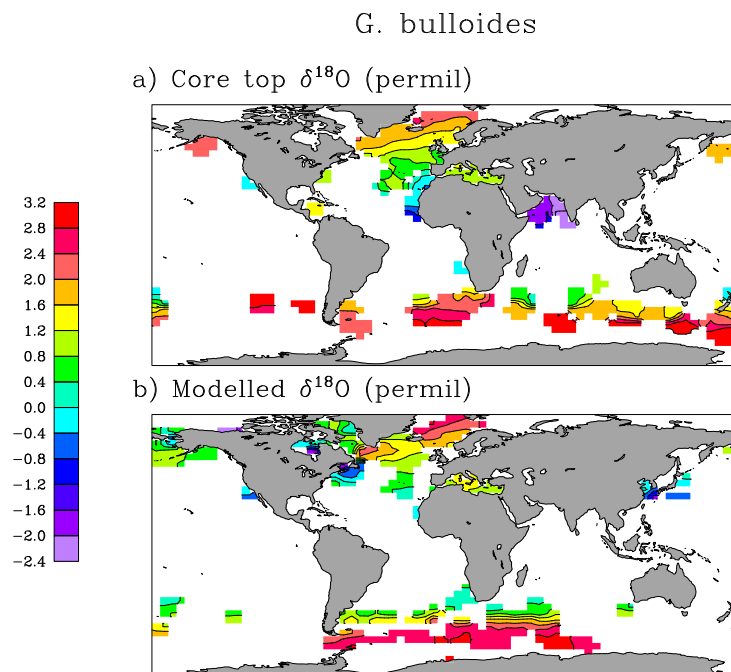


Figure 5. *G. bulloides*. Description as for figure 2, except that the modelled results are spliced from two different sets of parameters. The northern hemisphere results are from the results derived purely from considering the N. Atlantic coretops, while the southern hemisphere results are from the profile derived only from southern ocean coretops.

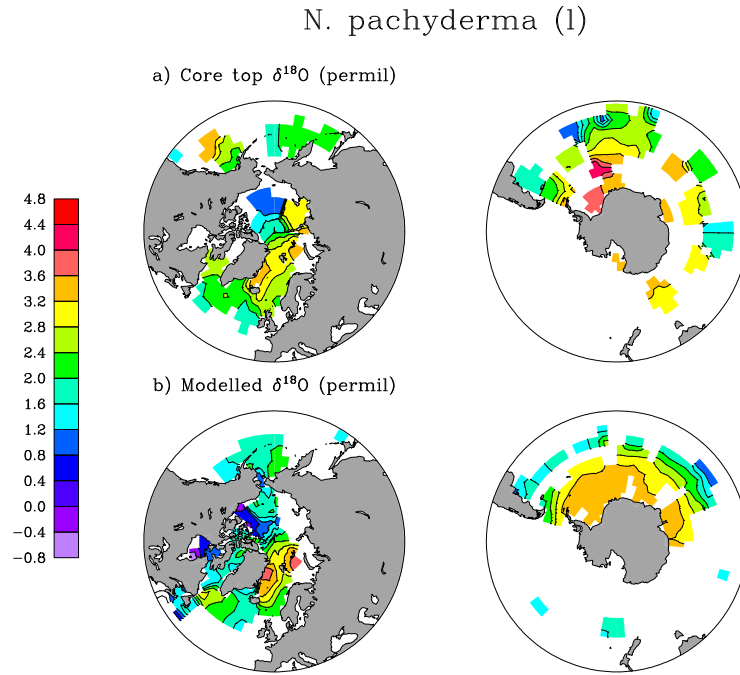


Figure 6. *N. pachyderma* (l). Description as for figure 2.

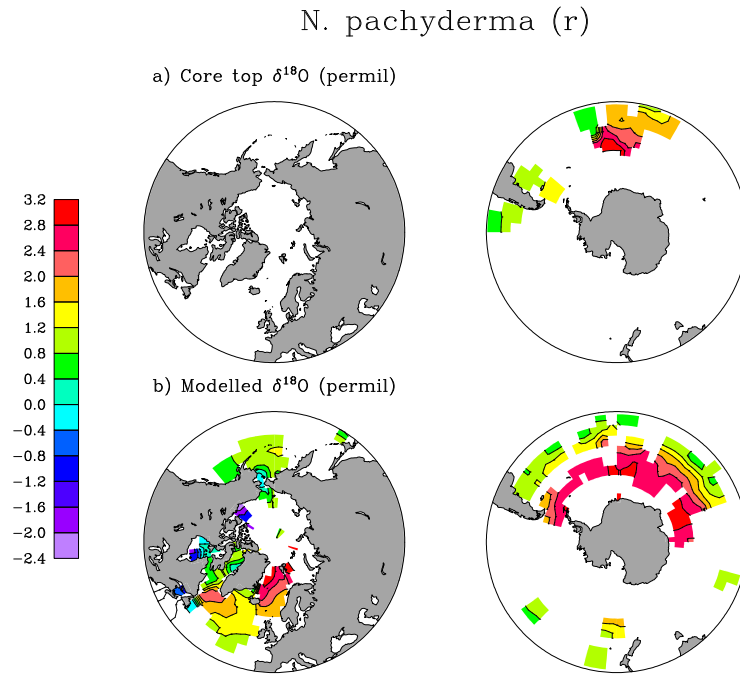


Figure 7. *N. pachyderma* (r). Description as for figure 2.

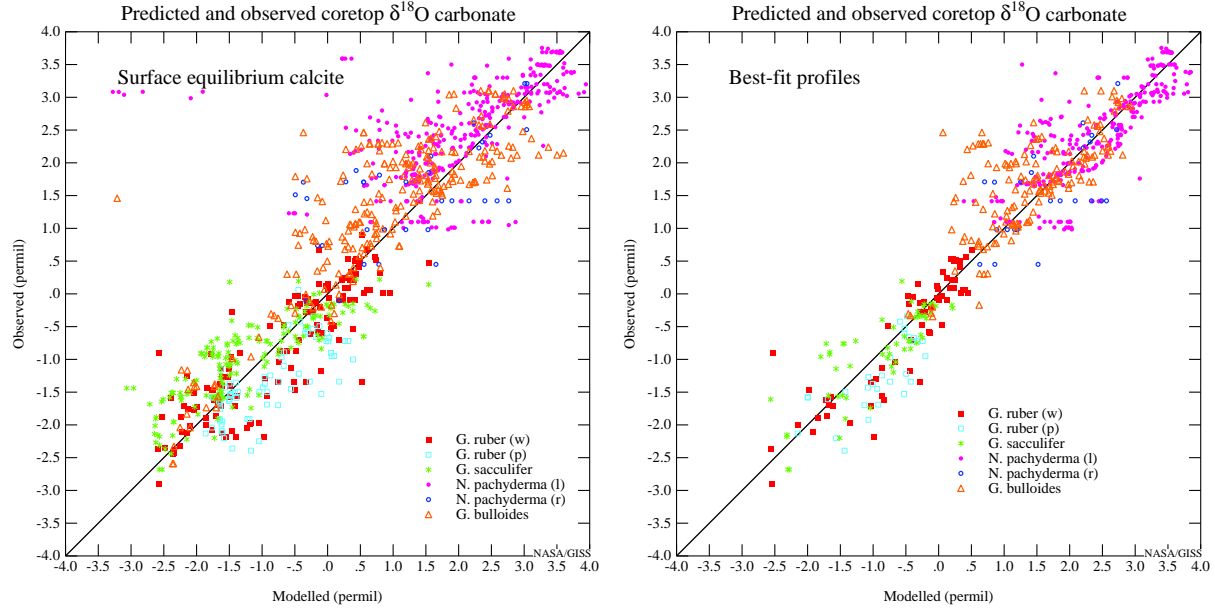


Figure 8. The predicted versus observed carbonate values for a) the generic model using only estimates of the surface equilibrium calcite, and b) the optimal ecological models derived here (Table 2). For the modelled values the standard deviation is about 0.53‰ over the entire range, compared with 1.2‰ for the generic model using surface-only equilibrium calcite values (the number of points in the surface only model is greater due to the greater amount of surface-only $\delta^{18}\text{O}_w$ data available compared with sub-surface profiles).